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Conceptual Uncertainties in Modelling the Interaction between Engineered and Natural Barriers of Nuclear Waste Repositories in Crystalline Rock

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Abstract:

Nuclear waste disposal relies on multi-barrier concepts that includes bentonite and the crystalline rock. Material contrasts across the interface between the engineered and natural barriers lead to complex interactions between these two subsystems. Numerical modelling combined with data is used to improve the understanding of rock-bentonite interactions and to predict the performance of this coupled system. While established methods exist to examine the prediction uncertainties due to uncertainties in input parameters, the impact of conceptual model decisions on modelling results is more difficult to assess. An SKB Task Force project facilitated such an assessment, as 11 teams used different conceptualisations and tools to analyse the Bentonite Rock

	Interaction Experiment (BRIE) conducted at the Äspö Hard Rock Laboratory. The exercise revealed that prior system understanding and features implemented in the simulators affect the processes included in the conceptual model. The exercise identified conceptual uncertainties that led to different assessments of the relative importance of the engineered and natural barrier subsystems. The range of predicted bentonite-wetting times encompassed by the ensemble results were considerably larger than the ranges derived from individual models. This is a consequence of conceptual uncertainties, demonstrating the relevance of using a multi-model approach that involves alternative conceptualizations.
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Conceptual uncertainties in modelling the interaction between engineered and natural barriers of nuclear waste repositories in crystalline rock

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Running title: Conceptual model evaluation of bentonite-rock interaction

Abstract: Nuclear waste disposal in geological formations relies on a multi-barrier concept that includes engineered components—which in many cases includes a bentonite buffer surrounding waste packages—and the host rock. Material contrasts and gradients across the interface between the engineered and natural barriers lead to complex interactions between these two subsystems. Numerical modelling combined with monitoring and testing data can be used to improve the overall understanding of rock–bentonite interactions and to predict the performance of this coupled system. While established methods exist to examine the prediction uncertainties due to uncertainties in input parameters, the impact of conceptual model decisions on the quantitative and qualitative modelling results is more difficult to assess. An SKB (Swedish Nuclear Fuel and Waste Management Co.) Task Force project facilitated such an assessment, as 11 teams used different conceptualisations and modelling tools to analyse the Bentonite

Rock Interaction Experiment (BRIE) conducted at the Äspö Hard Rock Laboratory in Sweden. The exercise revealed that prior system understanding along with the features implemented in the available simulators affect the processes included in the conceptual model. For some of these features, sufficient characterization data are available to obtain defensible results and interpretations, while others are less supported. The exercise also helped identify conceptual uncertainties that led to different assessments of the relative importance of the engineered and natural barrier subsystems. The range of predicted bentonite-wetting times encompassed by the ensemble results were considerably larger than the ranges derived from individual models. This is a consequence of conceptual uncertainties, demonstrating the relevance of using a multi-model approach that involves alternative conceptualizations.

The safety of radioactive waste disposal in geologic formations is partly determined by a science-based assessment of the barrier functions of the entire repository system, which includes engineered and natural components. In most disposal concepts, the Engineered Barrier System (EBS) consists of a suitably conditioned waste form enclosed in canisters, which are embedded in a buffer material emplaced in horizontal tunnels or vertical deposition holes. The EBS components are designed to protect the waste from mechanical and hydro-biogeochemical impacts that would lead to an early or substantial release of radionuclides from the repository to the host rock and its pore water. The host rock itself protects the EBS and retards the transport of radionuclides to the accessible environment. Both the engineered and natural barrier systems act together; they also interact with each other across the interface between the buffer and the wall of the tunnel or the deposition hole that contains the waste. In what follows, we consider a bentonite buffer in a deposition hole excavated from a fractured granitic host rock located deep below the water table.

The behaviour of each element of the EBS and natural system needs to be characterised, understood, and (to the extent possible) predicted for the duration of the compliance period. Numerical modelling is a key tool used to test hypotheses, to design laboratory and field experiments, to analyse data, and to make predictions about the system behaviour for a variety of scenarios. Many siting and repository design decisions are supported by the improved understanding or quantitative assessments that are based—in part—on numerical modelling.

A computer model is a numerical implementation of a mathematical description of our current conceptual understanding (see, e.g., NRC 1996). This conceptual model is an abstraction and thus simplified representation of the actual system. Predictions made with such a model necessarily contain errors, defined as systematic differences between the model output and the corresponding true system behaviour. Apart from the fact that the true system behaviour cannot be perfectly known but only approximately gleaned from sparse, noisy, and potentially erroneous data, modelling errors can be considered tolerable as long as the model fulfils its purpose of improving system understanding or making a prediction with an acceptable uncertainty range.

Errors and uncertainties in model predictions stem from multiple sources. Errors from numerical approximations (e.g. truncation and discretization errors) and uncertainties in input parameters are two sources of prediction uncertainties that are well studied. The former is typically quantified by comparing simulation results with analytical solutions, whereas the latter is examined by sensitivity-based or sampling-based error propagation methods. The resulting uncertainty ranges, however, may be optimistic, as they do not include potential errors in the underlying conceptual model.

The often-dominant impact of the conceptual model on simulation results is widely acknowledged; some illustrative examples are described in Bredehoeft (2003). As a consequence, various methods have been proposed to (1) gain confidence in the appropriateness of the chosen conceptual model; (2) rank the performance of alternative conceptual models; (3) identify plausible models or select the most appropriate model; (4) average multiple models to obtain consensus predictions; (5) quantify the sensitivity of model outputs to changes in the conceptual model; (6) quantify uncertainty in predictions as a result of conceptual model uncertainty; and (7) guide future data collection and modelling activities.

Papers published in the scientific literature range from philosophical discussions (e.g. Pappenberger and Beven 2006) to qualitative descriptions (e.g. Marivoet *et al.* 1997), empirical studies (e.g. Bredehoeft 2005), and quantitative theories (e.g. Neuman 2003). In hydrogeology, most of the literature related to conceptual uncertainty revolves around the generalised likelihood uncertainty estimation (GLUE) method (Beven and Binley 1992), Bayesian model averaging (Draper 1995), the use of model selection criteria (Ye *et al.* 2008), and combinations thereof (Rojas *et al.* 2010; Ye *et al.* 2010; Singh *et al.* 2010). A few papers describe conceptual model comparison studies for specific application areas, including nuclear waste isolation (Baca and Seth 1996; Marivoet *et al.* 1997; Sawada *et al.* 2005; Rutqvist *et al.* 2009; Hudson *et al.* 2009; Reeves *et al.* 2010; Li *et al.* 2011). Many more studies focus on benchmarking and code comparisons (e.g. Oldenburg *et al.* 2003; Pruess *et al.* 2004; MDH 2005; Steefel *et al.* 2014); they often do not fully include uncertainties caused by the process of developing a conceptual model from available information. Conceptual model uncertainty has been discussed as part of international code and model comparison projects, such as INTRAVAL, INTRACOIN, HYDROCOIN, PSACOIN, DECOVALEX, CO2BENCH, and SSBENCH.

A review of the literature leads to the following observations:

(1) Identification of the true (or even most likely) conceptual model is considered fundamentally impossible (e.g. Oreskes *et al.* 1994);

(2) Multiple (if not many) conceptual models need to be developed (or conceptual aspects of a model need to be parameterised) for a suitable analysis;

(3) Measured data are often required to calibrate the model or to evaluate its performance (e.g. Pappenberger *et al.* 2015);

(4) Estimates of prior model probabilities and input parameter uncertainties as well as their impact on predictions are often required as part of a formal conceptual model uncertainty analysis (e.g. Neuman 2003);

(5) A suitable likelihood measure needs to be defined and evaluated for each alternative conceptual model (e.g. Ye *et al*. 2008; 2010);

(6) Most approaches involve computationally expensive Monte Carlo sampling methods

(e.g. Rojas *et al.* 2010);

(7) Model performance is most often evaluated in the calibration rather than prediction space (e.g. Poeter and Andersen 2005);

(8) Correlations among alternative conceptual models are seldom accounted for, with the notable exception of Sain and Furrer (2010); as correlations among alternative conceptual models tend to be very strong, simple methods (such as bootstrapping) may not be employed.

Many of the requirements implied in these observations make it difficult to formally evaluate conceptual model uncertainties. In this paper, we present an effort to examine conceptual model uncertainties by comparing a number of alternative models that were developed to better understand the interaction between the engineered and natural barrier systems of a nuclear waste repository. The study was conducted as part of Task 8 of the Swedish Nuclear Fuel and Waste Management Co. (SKB) Task Forces on Engineered Barrier Systems (EBS Task Force) and on Ground Water Flow and Transport of Solutes (GWFTS Task Force).

SKB Task Force

The SKB Task Force is a forum for international organizations to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock and engineered barrier systems. The SKB Task Force formulates tasks that are addressed by multiple teams of modellers. In particular, the overall objective of Task 8 was to obtain a better understanding of the hydraulic interaction between the near-field natural host rock and the engineered bentonite buffer in a deposition hole. Eleven organizations participated in Task 8; they are listed in Table 1.

Table 1. *Organizations participating in SKB Task Force modelling of Task 8*

Organization	Acronym	Country
Amec Foster Wheeler	Amec	UK
Clay Technology AB	Clay Tech	Sweden
Computer-aided Fluid Engineering and Golder Assoc.	CFE-Golder	Sweden
Gesellschaft für Anlagen- und Reaktorsicherheit gGmbH	GRS	Germany
Japan Atomic Energy Agency	JAEA	Japan
Korea Atomic Energy Research Institute	KAERI	Korea
Los Alamos National Laboratory	LANL	USA
Royal Institute of Technology	KTH	Sweden
Stockholm University	SU	Sweden
VTT Technical Research Centre of Finland Ltd	VTT	Finland
Technical University of Liberec	TU Liberec	Czech Rep.

With the specific goal to examine how the characteristics of the fractured host rock affect the wetting of the compacted bentonite used as buffer material in a deposition hole, Task 8 targeted a configuration representing the Bentonite Rock Interaction Experiment (BRIE), which was performed at the Äspö Hard Rock Laboratory, located near Oskarshamn in southeastern Sweden. The BRIE addresses the hydraulic interaction between compacted bentonite and the near-field fractured host rock. The experiment is located in the short TASO tunnel at approximately 400 m depth. The TASO tunnel is hosted in rather massive, medium-grained diorite, with some more gabbroic volumes in addition to volumetrically significant granitic dykes and smaller, irregularly shaped granitic intrusions. Vertical test boreholes (76 mm diameter) were drilled for initial characterization and screening. Inflow to the holes was measured and two of the boreholes were then widened (to represent surrogate deposition holes) to accommodate pre-compacted and instrumented bentonite blocks as shown in Fig. 1. Prior to emplacement the inflows to the 300 mm-diameter boreholes were characterised. The BRIE site, experimental procedures and results are fully documented in Fransson et al. (2017).

The BRIE field experiment is complemented by a radial water-uptake laboratory test as shown in Fig. 2 (further details can be found in Fransson et al. 2017). The Task 8 modelling work and the BRIE experiments are interlinked in that the modelling is in part used to support the design of the laboratory and field experiments, whereas the experiments provide characterization data, modelling scenarios, as well as data that are further used to evaluate the conceptual appropriateness, explanatory capability, and predictive power of the numerical models.

Fig. 1. The BRIE site in the TASO tunnel: drilling of the 300 mm boreholes (left), emplacement of the 3 m bentonite blocks (middle), extraction of bentonite blocks after 17 months (right) (source: Fransson *et al.* 2017).

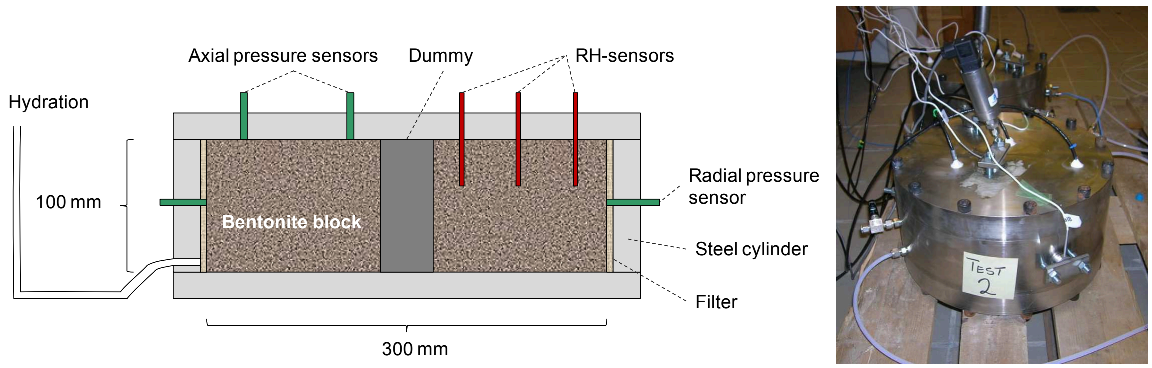


Fig. 2. Schematic and photograph of the BRIE water-uptake test. Water is introduced via the outer cylindrical filter. The 100 mm bentonite block is identical in material to the stack of blocks emplaced in the BRIE in situ experiments (Fig. 1) (source: Fransson *et al.* 2017).

The interaction between the host rock and the engineered barrier system involves complex two-way processes. Their understanding and predictability critically depends on the underlying conceptual model, the available characterization data, the geologic and engineered features represented, the hydrological, mechanical, and geochemical processes considered, and the details of their implementation in a numerical model. Moreover, it is essential to assess the impact of each model element on the results of interest, and how they in turn affect the conclusions and recommendations derived from these numerical studies. To examine the robustness and uncertainties of the models, different concepts and modelling approaches were developed by several modelling groups (Table 1) that addressed the same questions related to the overall objectives. The intention of this strategy is that the combined results of all modelling studies are likely to increase our understanding of the features and processes governing bentonite-rock interaction, and that a cross-comparison of the different groups' findings can provide insights into the variability and uncertainty inherent in such analyses.

The key elements of the natural and engineered system investigated by the Task 8 modelling groups are shown in Fig. 3, which also summarises some of the main issues that needed to be addressed. The modelling groups needed to make (among others) the following conceptual decisions:

The model needs to cover a finite region of granitic rock that contains multiple engineered underground structures. The crystalline rock contains fractures and other discrete features on multiple scales. They may be represented using either (a) a continuum porous-medium model with effective properties, (b) a stochastic discrete fracture network (DFN) model, (c) a continuum model with large, discrete features implemented deterministically, (d) a DFN model with large, discrete features implemented deterministically, or (e) a hybrid model, combining continuum and discrete models, with fractures implemented deterministically or using stochastic methods. Specifically, fractures intersecting underground openings may be represented deterministically. Moreover, boundary conditions need to be specified at the outer model domain boundaries and the walls of underground openings. The impact of the TASO tunnel must be accounted for, as near-field pressure drawdown has developed due to long-term water seepage into the tunnel, which may be affected by evaporation.

Similarly, the small-diameter probing holes need to be represented and the relevant hydraulic testing procedures simulated. Larger-diameter (300 mm) surrogate deposition holes need to be included; these deposition holes are initially open but eventually filled with bentonite. Skin zones around all underground openings may have developed because of mechanical effects, dry-out due to evaporation, desaturation due to suction by the bentonite, or other mechanisms. In particular a more fractured excavation damage zone (EDZ) was identified in the floor of the tunnel. Inflow into open holes needs to be simulated, possibly accounting for a seepage face caused by capillary pressure effects.

Inflow into open or bentonite-filled holes occurs through discrete features and through the rock mass between these features. Hydraulic properties and connectivity of the fracture network determines the amount of water being supplied to the fractures intersecting the open or bentonite-filled holes. Interactions between the fractured rock and the bentonite occur through an interface between the surrogate deposition hole wall and the bentonite. Feedback mechanisms between the two systems across this interface may be relevant. Capillary and pressure forces drive water entering the bentonite; water imbibition is potentially affected by local desaturation and other skin effects. Finally, water that entered the deposition hole non-uniformly through the interface is redistributed within the bentonite.

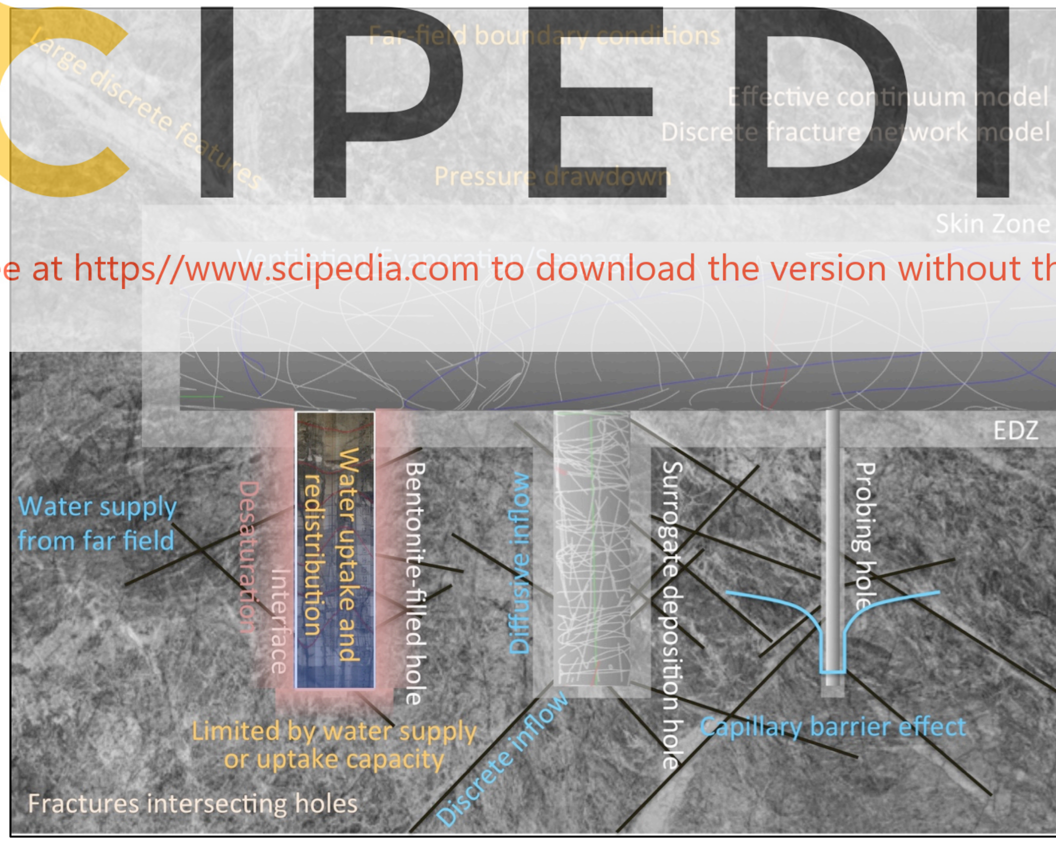


Fig. 3. Schematic of key system elements, processes, and modelling issues related to the interaction between fractured diorite and a bentonite-filled surrogate deposition at the Äspö Hard Rock Laboratory, Sweden.

Task 8 was structured into subtasks. Following a simple scoping calculation, the BRIE experiment was modelled in four stages with increasing complexity, incorporating more experimental data as they became available. All subtasks involve the modelling of both flow in the fractured bedrock and inflow into surrogate deposition holes that are either open or backfilled with bentonite. In addition, the water-uptake test (WUT) provided additional characterization data and insights into the wetting behaviour of the bentonite (Fransson *et al.* 2017); separate numerical models were developed to analyse the WUT data and to get confidence in the representation of the bentonite in the models developed for the BRIE.

Objectives

The objectives of this paper is to describe how the results of the Task 8 modelling study may have been affected by decisions about the underlying conceptual model, i.e., to address the question to which degree the general understanding of bentonite-rock interaction as well as specific predictions of bentonite wetting vary due to conceptual model uncertainty. This is the description of a case study rather than the development of new metrics to compare alternative conceptual models.

Approach

Each of the modelling groups (see Table 1) developed a conceptual and related numerical model of the system, based on the objectives and information provided in the SKB Task Force description of Task 8 (Vidstrand *et al.* 2017). While each group focused on a single conceptual model, the project as a whole produced results that are based on a suite of alternative conceptual models. These models have different levels of accuracy as well as overlapping (but not identical) input spaces, which arise from sharing the task description and some common aspects of the underlying conceptual understanding. Synthesizing the results of these alternative conceptual models requires some evaluation of the prediction uncertainty that includes conceptual, parametric, and numerical errors and their correlations. While no model comparison based on formal criteria is attempted, the discussion is intended to be as specific as possible in that it focuses on the repository subsystem at hand, the hydrogeological features of that subsystem, the numerical models that were developed as part of Task 8, and the target predictions these models were asked to deliver.

To guide such a discussion, specific information from each of the modelling groups was collected as the basis for a comparative analysis. Most of the requested information consists of a concise and complete documentation of each modelling group’s system understanding, the features implemented in their models, the explicit and implied assumptions made during model development, and the modelling groups’ assessment of the validity and uncertainty of these assumptions. In addition, results from the sensitivity analyses conducted by most modelling groups and more general evaluations of the quality of model predictions were summarized. These descriptions were supplemented with results from numerical simulations or estimated measures of prediction uncertainty.

It is understood that conceptual model errors are an inherent part of numerical modelling, as building a model involves an abstraction process during which certain aspects of the real system are simplified. To become more aware of this abstraction process and to highlight the further simplifications made when implementing the conceptual model into a numerical model, the concept of a “reified model” (Goldstein and Rougier 2009) was used. A reified model is the “best conceivable model” a user would develop without being constrained by computational limitations. Defining such a hypothetical model allows one to separate potential errors made during the abstraction step and those made during the implementation step. Note that the difference between the true system and the reified model reflects our incomplete knowledge of the system behaviour, whereas the difference between the reified model and the actual computer model used for an analysis reflects modelling limitations. The first discrepancy is fundamentally not knowable; modelling errors are (at least theoretically) knowable.

While Goldstein and Rougier (2009) introduced reified analysis as part of a Bayesian framework, the concept of a reified model is used here solely as a tool to clarify the relation between the computer model and the physical system. A questionnaire (Table 2) was developed to obtain a concise description of the physical system, the reified model and the model actually used for the study. In addition, questions related to the relative importance of conceptual and parametric model elements and their uncertainties were formulated to solicit information about the confidence the modellers have in their system understanding and the reliability of their model predictions. The completed questionnaires built the basis for understanding differences in conceptual models and differences in results and their interpretations, which is discussed below. The responses to the questionnaire were then discussed at a one-day workshop to identify key areas of consensus and disagreement.

Table 2. *Questionnaire soliciting input for comparative*

#	Topic	Question
True system, reified model, and actual model		
1	True system	Describe current system understanding, including hydrogeological features, processes, and conditions that are considered relevant to understand and predict the behaviour of the host rock, bentonite, and interface between them.
2	Reified model	Describe a hypothetical model that best represents the true system behaviour, specifically model features that are considered influential.
3	Actual model	Describe the features, processes, and conditions implemented in the actual model used to predict the behaviour of the repository subsystem, including assumptions, simplification, limitations, restrictions and constraints.
4	Alternative model	Describe alternative conceptual models considered viable to explain and predict true system behaviour, or to question or disprove the hypotheses examined with the actual model.
Input and prior uncertainties		
5	Prior uncertainties	Describe and quantify the state of knowledge or uncertainty about features that are included or excluded from the actual model.
Sensitivities		
6	Impact on understanding	Describe potential impact of model features on overall system understanding.
7	Impact on predictions	Describe and quantify impact of model features on specific model predictions.
Ranking		
8	Ranking of features	Rank model features, omissions, simplifications, and assumptions according to their potential impact on overall system understanding and numerical model predictions.
9	Weighting of features	Assign weights to the ranked model features, omissions, simplifications, and assumptions to reflect the order of magnitude of the expected impact.
Prediction uncertainty		
10	Uncertainty in understanding	Describe the degree of confidence you have about the overall system understanding given conceptual uncertainties and their impact on that understanding.
11	Uncertainty in predictions	Describe the degree of confidence you have in your model predictions given conceptual uncertainties and their impact on these predictions.

Calibration and prediction		
12	Data uncertainty	Assess the quality of the BRIE and water uptake test (WUT) data, i.e., uncertainties and potential systematic errors.
13	Expected residuals	Describe which component of the measured data the model is expected to reproduce and predict (e.g., order-of-magnitude behaviour, average value, general trend, low-frequency fluctuations, high-frequency fluctuations, all details except measurement error, all details including systematic component of measurement error).
14	Prediction	Describe how well your model predicted the system behaviour observed during the BRIE and WUT experiments.
15	Calibration	Describe how well your model reproduced the system behaviour observed during the BRIE and WUT experiments.
Specific predictions		
16	Predictions	Provide the model-predicted best-estimate value of inflow into the open probing holes. Provide the model-predicted best-estimate saturation values at the time of dismantling. Provide the model-predicted best-estimate values of the time for bentonite resaturation to 95%.
17	Uncertainty	Provide the uncertainty (range or distribution) of these predictions based on parametric uncertainties in the actual model used for these predictions. Describe which parametric uncertainties are considered in this assessment.
18	Conceptual uncertainty	Describe the uncertainty of these predictions accounting for conceptual model uncertainties. Describe which conceptual uncertainties are considered in this assessment.
General assessment		
19	Under-standing	Describe the main improvement in system understanding gained by performing Task 8.
20	Change in uncertainty	Describe how uncertainty has changed as new data from BRIE and WUT were incorporated into the model.
21	Conceptual uncertainty	Describe the degree to which the current conceptual understanding is believed to represent the behaviour of the true system.
22	Model uncertainty	Describe the degree to which the current numerical model is believed to represent the behaviour of the true system.
23	Key uncertainty	Describe which aspect of the conceptual or numerical model is the main source of insufficient system understanding and prediction uncertainty.
24	Research plan	Describe how uncertainty in this main aspect could be reduced by collecting additional information or data, and what specific changes to the actual model could be made to improve system understanding and to reduce predictive uncertainty.

Conceptual models

This section provides a brief description of the different conceptual models developed by the modelling groups listed in Table 1. While presented with a common description of the system and the questions to be addressed, the modelling groups had the leeway to develop their own conceptual and numerical models using the software of their preference. Some of the features and processes considered relevant were described above and illustrated in Fig. 3. A large number of conceptual decisions needed to be made; some of the major decisions are discussed in the following subsections.

Physical processes

The main processes to be considered included fluid flow through fractured rock and imbibition into partially saturated bentonite. To limit the scope of the Task 8 modelling studies, the task description did not demand the use of complex, coupled models. For example, it was decided to disregard thermal and geochemical processes and their multifaceted interactions despite their likely impact on the system behaviour in an actual repository for heat-generating waste. Ignore thermal effects in the modelling also followed the choice to design BRIE as an isothermal test. Note that Gens *et al.* (2009) describe a full-scale in situ heating test of a bentonite buffer (FEBEX). Some modelling groups included the expected effects of coupled mechanical processes on near-borehole conditions by specifying skin zones. Flow processes were represented using one of the following governing equations:

Saturated flow using Darcy's law. Darcy's law was used to simulate flow through porous media for both the fractures and (if included in the model) the rock mass in between fractures. The underlying assumption of fully liquid saturated conditions ignores the potential desaturation of the formation near the bentonite-rock interface. A separate model is used to simulate the partially saturated bentonite.

Diffusion equations. Unsaturated flow in the bentonite was modelled using a diffusion equation with a nonlinear, saturation-dependent diffusion coefficient. One group developed a model that accounted for diffusive flow of vapour in the pore space as well as that of interlamellar water.

Richards' equation. Flow of water under partially saturated conditions was modelled using Richards' equation, which accounts for relative permeability and capillary pressure effects of the liquid phase, but ignores the presence of a viscous, compressible, and dissolvable gas phase.

Two-phase flow formulation. A two-component (water and air), two-phase (liquid and gas) formulation was used to account for flow and potential trapping of the gas initially present in the bentonite.

Simplified saturation method. One modelling group developed a method referred to as simplified saturation method, in which the storativity term in the balance equations for saturated flow is modified to account for the increase in water storage volume available under partially saturated conditions.

It should be noted that the differences between these formulations are relatively minor, specifically in comparison to uncertainties in their parameters, the high spatial variability in properties, and the potential effects of thermal, mechanical and geochemical processes.

All models are relatively simple. They are based on Darcy's law with static and non-hysteretic relative permeability and capillary pressure functions. This simple model was considered applicable to simulate fluid flow in swelling clays, fractures, fracture zones, and tight background rock, although the model choice also reflects the intention of the task to avoid complex coupled models.

The physics of fluid flow through swelling clay is less well established. Most models used in Task 8 were based on standard balance equations describing two-phase advective flow through porous media, driven by viscous and capillary forces. An alternative model considered diffusive water transport in two separate continua – the pore space and the interlamellar space – coupled by hydration. The resulting mathematical equations are similar to the Richards equation with a saturation-dependent hydraulic diffusivity (Kröhn 2016). Despite the similarities in the governing equations, the underlying physical models and their related conceptual uncertainties remain different.

Fractured rock representation

Fractures on various scales are likely to dominate groundwater flow in the bedrock, inflow into open and bentonite-filled deposition holes. How to appropriately represent individual fractures or the fracture network as a whole was thus a critical conceptual modelling decision.

The task description (Vidstrand *et al.* 2017) provided a detailed description of the geometry of underground openings (tunnels and boreholes) and the known, large hydrogeological structures in the BRIE area. Smaller-scale fractures were described by means of stochastic parameters. Fracture trace maps were made available, showing the intersection of fractures with tunnels and deposition holes. After dismantling of BRIE, the so-called bentographs (photographs of wetting patterns imprinted on the bentonite surface; see Fig. 7 below and Dessirier *et al.* 2017) provided an additional, detailed view of discrete, water-conducting features at the wall of the deposition holes.

The modelling groups approached the problem of how to include the effect of a large number of fractures into the numerical model in different ways, arriving at different alternative conceptual models, which in turn led to different emphases of the modelling studies and—most importantly—different conclusions. The approaches used included:

Homogeneous, effective continuum model. Continuum porous-medium models with effective parameters were used mainly to demonstrate that such an approach would oversimplify the complexity of the system and lead to unreasonable results.

Classic discrete fracture network model. Discrete fracture network (DFN) models were used by multiple modelling groups, albeit in different ways and for different purposes. The direct translation of the stochastic information of fracture networks from the task description yielded classic DFN models (see Fig. 4a), whereby multiple realisations of fracture networks that honour these statistics were generated. Some modelling groups conditioned the networks on fracture trace maps, and/or changed the statistics to account for the assumptions that not all fractures conduct water. Classic DFNs neglect interaction with the rock mass that is in between the fractures. They also neglect the impact of fractures that were smaller than a cut-off value (e.g. that used for fracture mapping). While certain modelling groups chose to only include a subset of mapped fractures into the model to account for hydraulically inactive fractures, others refer to the bentographs as supporting their view that all mapped fractures are water-conducting and should thus be represented in the model. Finally, only fully saturated flow was considered in the rock.

Discrete fracture network model as basis for a stochastic continuum model. Multiple modelling groups generated DFNs that were then mapped onto a continuum grid. Effective continuum properties were determined (either based solely on geometry or by performing local upscaling flow simulations) and assigned to each computational grid block, arriving at a heterogeneous continuum model (see Fig. 4b). Different approaches were used to upscale and map fracture properties to the continuum scale. Grid blocks that were not intersected by a fracture were assigned background rock properties.

Hybrid discrete fracture network model and continuum model. Some modelling groups posited that the discrete inflows across the rock-bentonite interface critically determine bentonite wetting, whereas the details of the far-field fracture network are insignificant as long as the network provides connectivity from a sufficiently large water source to the near field. Based on this conceptualization, they developed a hybrid model in which the mapped fractures intersecting the deposition hole are deterministically implemented into the model, while the far field is presented as a homogeneous, effective continuum (see Fig. 4c).

Artificial fractures and skin zones. The large impact of the fractures intersecting the deposition holes prompted an *ad hoc* inclusion of "artificial fractures". Similarly, skin zones were introduced to account for potential changes in fracture and background rock properties near underground openings (see Fig. 4d).

The list above demonstrates the variety of models developed for the natural barrier system of Task 8, which provides a unique opportunity to study the impact of alternative conceptualizations on predictions and conclusions. The wide variety is noteworthy specifically since all models were based on the same, rather extensive set of fracture data provided in the task description.

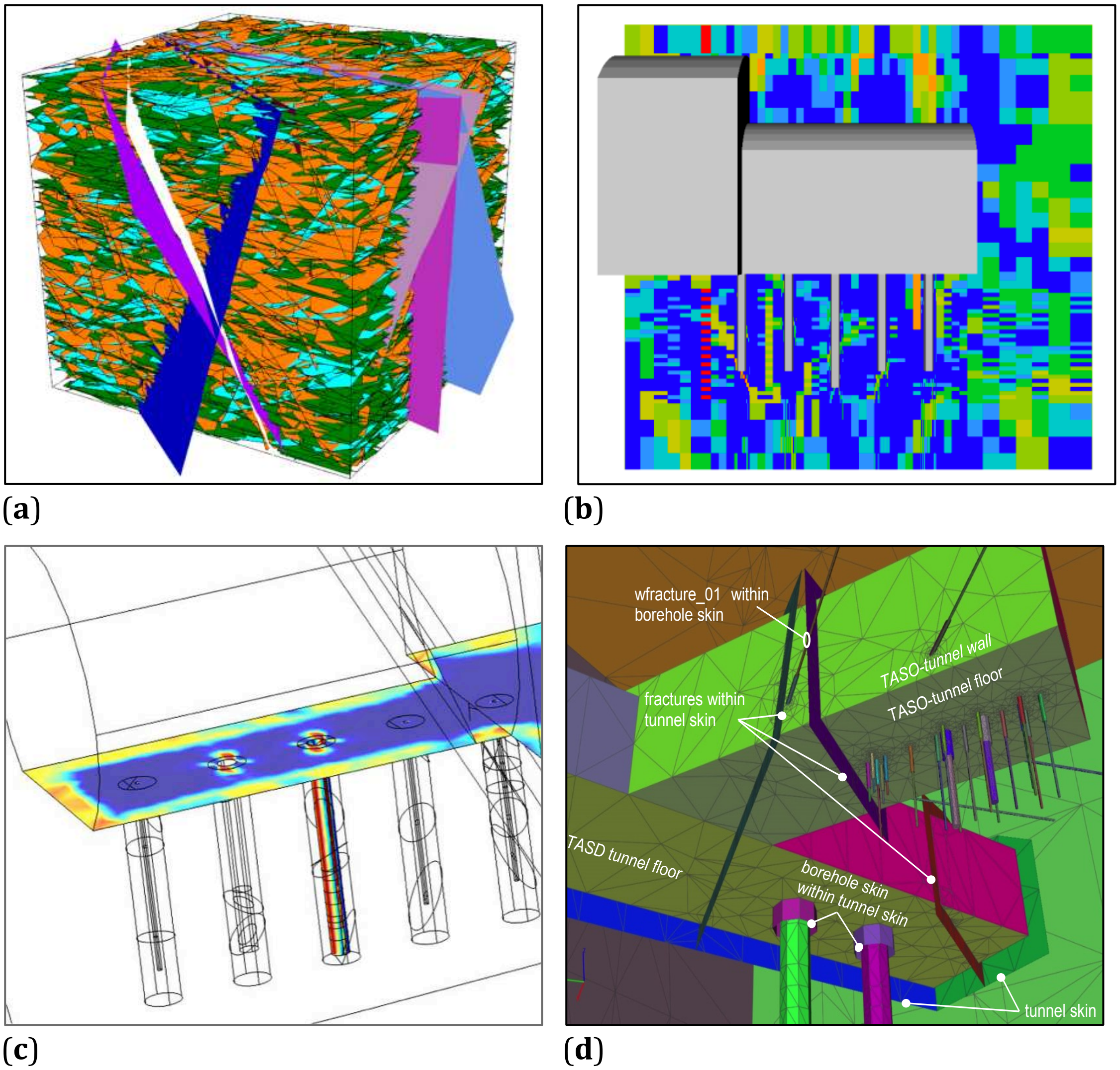


Fig. 4. Alternative representations of fractured rock: (**a**) classical discrete fracture network model, (**b**) heterogeneous effective continuum model with deterministic fractures around boreholes, (**c**) hybrid DFN-continuum model, and (**d**) model with artificial fractures and skin zones.

Bentonite representation

It is generally recognized that bentonite has complex coupled THMC behaviour (Wieczorek et al. 2017). The swelling properties of bentonite and specifically the relation between saturation, swelling pressure, absolute and relative permeabilities, and capillarity, are complex, non-linear functions that are difficult to measure experimentally and to implement into a numerical model. Impacts of ionic strength and temperature may also need to be accounted for. Further the emplaced bentonite was formed of multiple cylinders (Fig. 1) on a central tube, with the potential for preferential flows between cylinders.

Despite this complexity, all modelling groups treated the bentonite as a conventional, homogeneous porous medium, i.e., the use of classic flow equations and standard relative permeability and capillary pressure functions was considered appropriate for predicting bentonite hydration, acknowledging that the fitted capillary pressure curve accounted for other effects such as osmotic pressure. This confidence is mainly based on previous modelling of water uptake in bentonite (both in laboratory and field-scale experiments; Alonso *et al.* 1998; Gens *et al.* 2002; Vaunat and Gens 2005) and the success most modelling groups had in reproducing the data from the water-uptake test (Fig. 2). The WUT was a well-controlled laboratory experiment; the measured cumulative water uptake as well as saturation and relative humidity profiles were well matched by the models with minor adjustments of parameters.

Subsystem coupling

Task 8 required examination of the interaction between two, linked subsystems—the natural, fractured rock and the engineered, bentonite-filled deposition holes. These two subsystems can be combined by using a single model and a single simulator, or by coupling two models, each using a separate simulator.

Each modelling group chose one of the following coupling approaches that seemed appropriate for their conceptual model, available software, and research focus:

- *No coupling*: Information about the system state in the rock was transferred to the simulation of bentonite hydration in only a qualitative or conceptual way.
- *One-way coupling*: Information about the system state in the rock was transferred to the simulation of bentonite hydration in a quantitative manner (e.g., by specifying flow rates at the bentonite surface), but without accounting for feedback mechanisms between the two subsystems.
- *Iterative coupling*: State variables from one subsystem were specified as boundary conditions for the other subsystem; they were iteratively updated.
- *Full coupling*: The natural and engineered barrier systems were simulated using a single code and model, with all state variables solved simultaneously in a fully coupled system of equations.

The approach of separating processes and subsystems and studying them separately has certain advantages. It enables the use of specialized modules for each of the subsystems. For example, a DFN model can be developed to represent saturated flow in the fractured rock, and a continuum model can be developed to simulate two-phase flow in the bentonite. The strategy used to link the two models may provide an opportunity to implement or otherwise account for specific, difficult-to-simulate processes occurring at the interface between the two subsystems. The approach may also be computationally more efficient because (a) the system of fully coupled partial differential equations is smaller, (b) only the processes relevant for each subsystem need to be captured (e.g., two-phase flow conditions only need to be simulated in the bentonite, whereas fully saturated conditions can be assumed in the fractured rock), and (c) model domain scales and computational meshes can be independently optimized for the larger rock system and the smaller bentonite system.

On the other hand, treating the subsystems separately requires the development of a linking strategy between the two codes and models. This likely induces additional modelling errors that are difficult to detect or quantify. Specifically, the approach may not be able to account for feedback mechanisms between the two subsystems, unless an iterative coupling scheme is employed. Overall, it may make the approach less transparent.

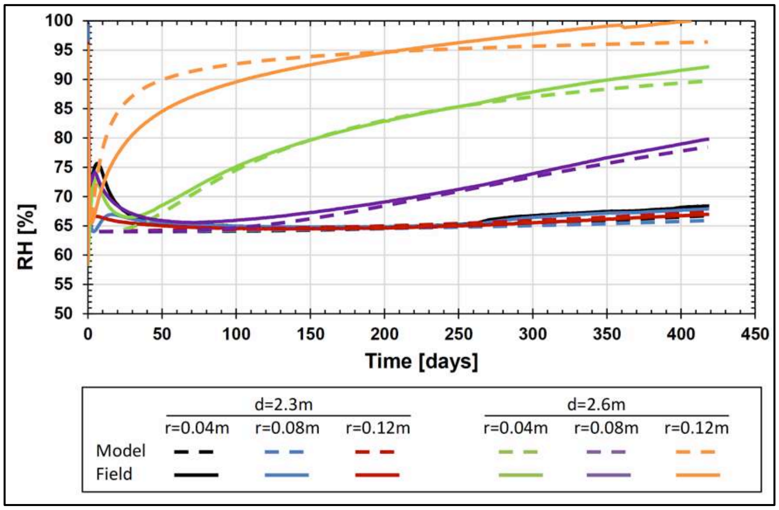
The approach in which both the natural and engineered barrier systems are simulated using a single coupled code and model, results in a fully integrated treatment of the entire system, which by design automatically accounts for feedback mechanisms between the two subsystems. This approach may be considered more transparent. However, a single model may not be able to optimally represent the specific processes in each of the subsystems. Moreover, processes at the interface between the two systems, which may be fundamentally different, may not readily be included. Finally, simultaneously solving all coupled governing equations, generally with nonlinear feedbacks, of the entire system is computationally demanding.

Model calibration and conditioning

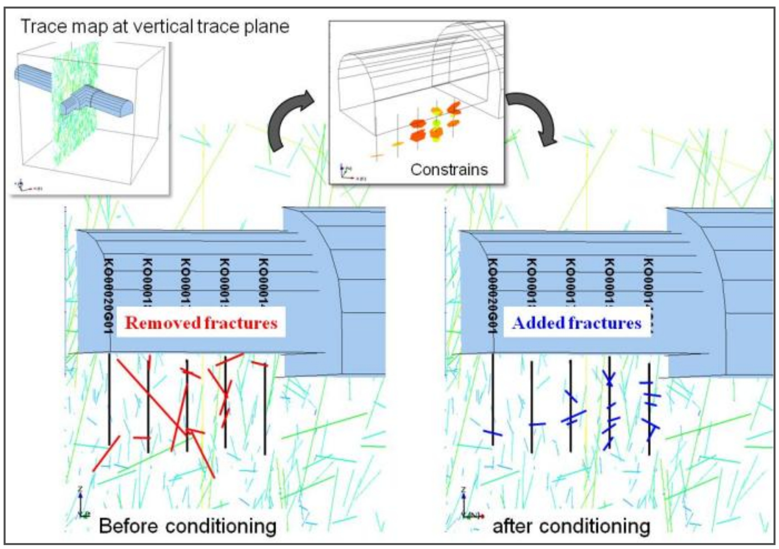
As a result of the abstraction process of developing a conceptual model, the governing equations necessarily contain effective parameters that are site specific and thus need to be determined by conditioning or calibrating the model using data from the BRIE. The estimation of effective properties also allows for partial compensation of errors in the conceptual model. Calibration is thus a key element of model development with considerable impact on the model's final ability to explain, reproduce and predict the system behaviour of interest.

The BRIE experiment provided characterisation data (such a fracture trace maps, hydraulic properties from core samples and *in situ* flow tests, inflows into tunnels and open deposition holes, pressures in packed-off borehole intervals, as well as relative humidities and water contents in the bentonite and near the borehole wall) that could be used for adjusting conceptual models and calibrating parameters. Furthermore, relative-humidity evolution data (Fig. 5a) were made available to the modelling groups during the course of the field experiment and were used to calibrate the models before the field experiment was dismantled. The features and parameters adjusted by the modelling groups included effective permeability of the fractured formation or rock mass between discrete fractures, skin zone permeability, and transmissivity of larger discrete features as well as the inclusion or removal of borehole-intersecting fractures. Moreover, DFN models were typically conditioned on fracture traces (Fig. 5b), and specific DFN realisations were selected on the basis of the match to observed inflow data (Fig. 5c). Data from the water-uptake test helped develop confidence in the representation of the bentonite's hydraulic behaviour (Fig. 6). Matching the data from sensors installed in the field and additional information obtained after dismantling of BRIE proved more challenging. Deviations between measured and calculated saturations and relative humidities were mainly attributed to inaccuracies in the relative positioning of sensors and fractures, uncertainty in fracture and background rock inflow rates, and experimental incidents with simplifications for the conceptual models.

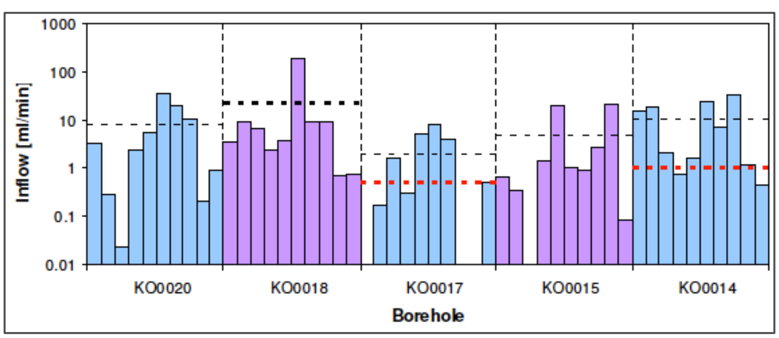
Most modelling groups evaluated the misfit between model output and measured data either visually or by comparing individual residuals. No formal calibration method was used, whereby an objective function (within either a maximum likelihood or Bayesian framework) is minimized or mapped out using an appropriate optimization or sampling algorithm. The main disadvantage of not using a formal approach is the lack of an *a posteriori* error and uncertainty analysis that would provide considerable insights into the system behaviour and potential ill-posedness of the inverse problem. Some modelling groups commented on ambiguities, goodness-of-fit, the structure of the residuals, and their confidence in the estimates obtained by the calibration effort.



(a)

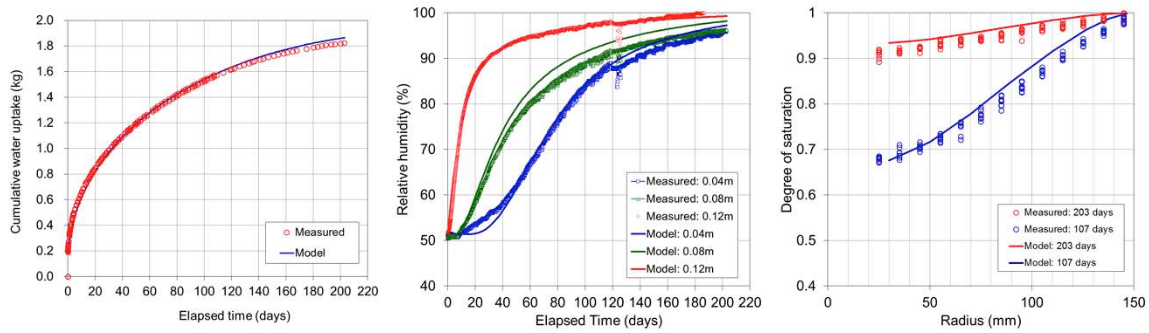


(b)



(c)

Fig. 5. Examples of the use of characterization and monitoring data: (**a**) reproducing relative humidity data; (**b**), conditioning of fracture locations and orientations; (**c**) selection of DFN realization that best reproduces inflow into open surrogate deposition hole.



(a) (b) (c)

Fig. 6. Comparison between measured and calculated (**a**) cumulative water uptake, (**b**) relative humidity, and (**c**) saturation for the WUT.

Software

The software tools used by the modelling groups ranged from well-established reservoir simulators to general-purpose PDE solvers to adaptations of existing tools for the incorporation of partially saturated conditions to new developments based on alternative formulations of the governing equations. In some cases, multiple tools were used, each dedicated to solving the flow problem particular to one of the two subsystems (fractured rock and bentonite).

It is acknowledged that the simulator available to a modelling group has an impact on the conceptual model in that its capabilities in part determines which processes are being considered, what features can be readily implemented, and how detailed the representation can be given its spatial discretization scheme and computational efficiency.

Simulation results

Simulating the evolution of pressures, flow rates, and saturations with a reference model and variants thereof allowed the modelling groups to better understand the factors affecting flow through the fractured rock, across the rock-bentonite interface, and within the bentonite during its hydration. Simulation results were visualized and qualitatively compared to observations from BRIE. For example, rightmost panel in Fig. 7 (referred to as a “bentograph”) was taken after dismantling of BRIE. It shows wetting patterns visible on the bentonite surface after having been in contact with the fractured rock for 17 months. The visual patterns were correlated to increased saturation, reflecting bentonite hydration (Dessirier *et al.* 2017). An example of corresponding numerical results is shown on the left panels. They represent one realization of a DFN model coupled to an unsaturated flow model for simulating bentonite wetting. The differences between the observed and simulated wetting patterns can be attributed to parametric and conceptual uncertainties. For example, the DFN model may have been conditioned to a geological fracture trace map that only identified some, but not all, water-bearing features.

Bentonite saturation distributions obtained with alternative modelling approaches are shown in Fig 8. A qualitative comparison of the patterns suggests that conceptual model decisions have a noticeable effect on the way water is carried to the interface and imbibed into the bentonite. Nevertheless, all models show that deposition holes excavated from fractured bedrock will experience discrete inflows and thus heterogeneous wetting of the bentonite. It becomes obvious that the location and orientation of the water-conducting fractures intersecting the hole determine wetting patterns and wetting times, and may compromise the homogenization function ascribed to the backfill material.

In addition to qualitative comparisons, specific predictions were made of the amount of water flowing into open probing and surrogate deposition holes, the relative humidity conditions within the bentonite, and the time needed to achieve a certain level of overall hydration.

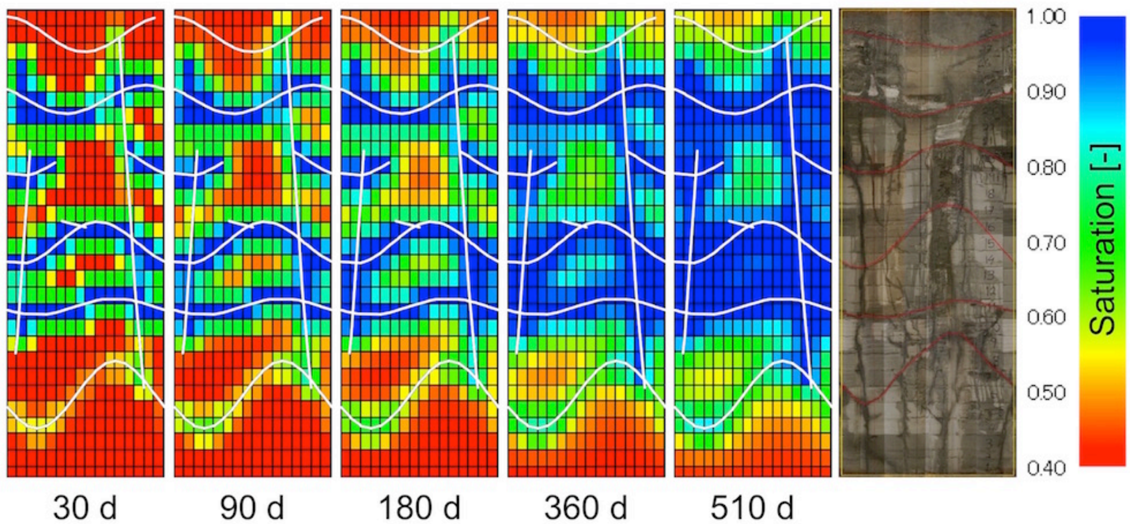


Fig. 7. Simulated (left) and observed (right) wetting patterns at the interface between fracture rock and the bentonite buffer.

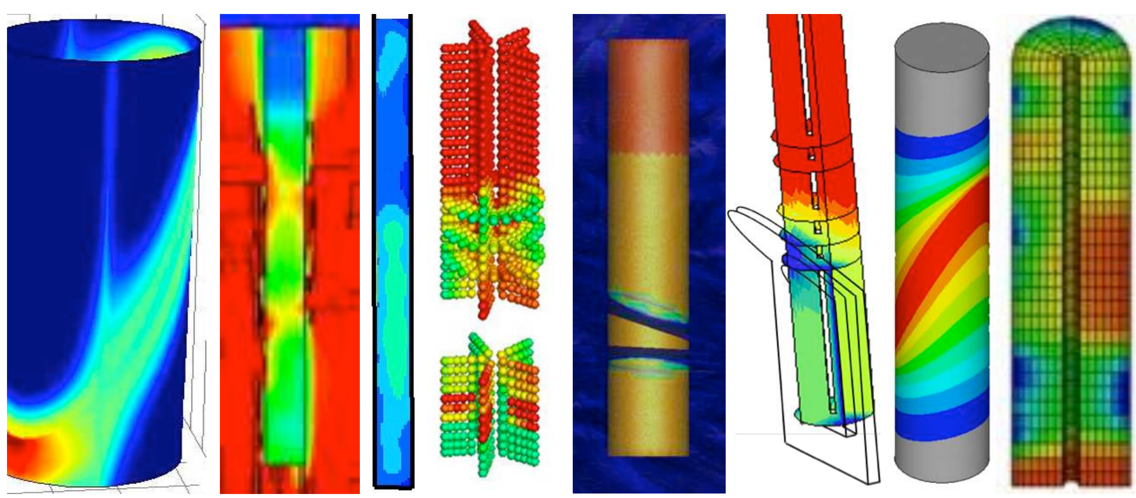


Fig. 8. Saturation distributions in bentonite calculated using different conceptual models.

Comparison and discussion

The fact that 11 modelling groups addressed a common set of questions using disparate data interpretations, conceptualizations, modelling approaches and simulation codes provided a unique opportunity for a comparison study. The purpose of such a comparison is not to identify the "correctness" of a prediction; instead, the goal is to obtain some insights into the variability in predictive results. More importantly, the various interpretations of data and simulation results and the evaluation of all findings improve overall system understanding and are likely to help identify areas where the knowledge can be considered sufficient or in need of further research.

We next present some of the similarities and differences in assumptions and results, before discussing how these differences affected the main conclusions reached by the modelling groups.

Conceptual models

The different formulations used to describe flow in bentonite and fractured rock all appear valid approximations, as demonstrated by successful reproduction of a reference solution that included radial wetting of a bentonite parcel intersected by a fracture, and the reproduction of the laboratory water-uptake test. Nevertheless, the choice of the conceptual model and associated governing equations appeared to have an impact on the research topic chosen for analysis, and the simulation results and conclusions. In particular, using a full two-phase formulation allowed for an analysis of gas trapping, which may be relevant when calculating the wetting time needed to (almost) reach complete saturation of the bentonite (Dessirier *et al.* 2014; 2015). Moreover, the impact of potential desaturation of the host bedrock could not be analysed when using a saturated flow model.

The modelling groups' conceptualisations also appear partly driven by their choice of simulation software, specifically the ability to generate stochastic fracture networks. Once this choice was made, however, the subsequent analyses were partly limited (e.g., to saturated flow without consideration of matrix or unmapped small fractures). This may have led to a bias in the conclusions. Conversely, DFN models were able to examine the spread of predictions as a result of spatial variability, randomness, and uncertainty in fracture characterisation.

The modelling groups that developed a hybrid approach generally went through a detailed examination of conceptual issues based on available data and their system understanding. They assessed the potential influence of each natural feature and related modelling component, and discussed the appropriateness of the simplifications they made (specifically the decision not to use a DFN in the far field). This deliberate consideration of the balance between fidelity and computational efficiency generally led to well-documented, defensible conceptual models.

The calibration process had the following notable outcomes. The accurate reproduction of the water-uptake test data—with little need for parameter adjustments—gave considerable confidence in the way the bentonite was represented and parameterised in the model. The confidence in the bentonite model helped reduce ambiguities when analysing data from BRIE dismantling and the bentographs. Key uncertainties in model predictions were almost exclusively attributed to uncertainties in the geometry, connectivity, and hydrogeological properties of the fractured rock.

As parameters are related to the chosen conceptual model, adjusting them to match the observed data necessarily led to a changed perspective of the system. The corresponding conclusions, however, may be biased due to limitations in the conceptual model. Specifically, the relative impact of fractures and the rock mass on bentonite hydration depends on the parameterization of the rock formation. A DFN model that does not account for flow through the rock mass compensates for that fact by further increasing the transmissivity of the fracture network during the calibration process, thus giving rise to the notion that background rock flow is insignificant. Conversely, a model that overestimates background rock flow due to an artefact in the upscaling procedure may underestimate the importance of the fractures for bentonite wetting. Whereas such errors would be negligible in predictions of large-scale inflows to various sections of the main tunnel at the Äspö HRL, they may need attention at the smaller scales relevant for deposition holes, since deposition holes may be placed deliberately in intact regions of the rock that contain low-conductive fractures only (Tirén *et al.* 1999).

To make DFN models better reproduce observed data, several adjustments of a different nature were made. These adjustments included (a) conditioning the network to known fracture traces in deposition holes, (b) calibrating fracture transmissivities and other properties, and (c) picking the realisation that best matches observed inflow data. This flexibility in adjusting different DFN model components makes it relatively easy to match observed data. At the same time, it becomes difficult to avoid ambiguities and non-uniqueness that is inherent in an underdetermined inverse problem. Furthermore, it is difficult to see which aspect of the fracture network (e.g., its geometry, or hydraulic properties, or spatial randomness) most critically affects bentonite hydration. On the other hand, the stochastic framework adopted by DFN modellers allowed them to examine the rather wide spread of results that is solely due to irreducible variability in the statistical descriptions of fracture network structure.

The methods used to calibrate and condition a DFN (or hybrid models that are supported by a DFN) are interesting, as they address the difficult issue of concurrent parameter estimation and model structure identification. They also raise some fundamental questions about the appropriate level of model complexity, the relation between uncertainty and variability, and the relative importance of geometric and hydrogeologic properties.

Predictions

One purpose of numerical simulations is to make quantitative predictions of a future system behaviour that cannot be readily inferred from historical data or from studying analogue systems. The numerical models developed as part of Task 8 were used to calculate a full set of independent and derived state variables at a large number of points in space and time. A small subset of these model outputs was identified as representing the system behaviour of interest, i.e., the quantities that most directly speak to the modelling objectives of understanding the exchange of water across the bentonite-rock interface and bentonite wetting, which may be criteria used for characterising the suitability of deposition holes. These outputs are termed "performance measures", and they naturally offer an opportunity to quantitatively compare the outcome of alternative conceptual and numerical models. The performance measures of interest are the inflows into probing and surrogate deposition holes as well as the time for hydrating the bentonite to a specific saturation level (typically 95%). The following subsections summarize the values and (if reported) uncertainty ranges obtained by each of the modelling groups.

Inflow into open boreholes was selected as a performance measure because it may be used as a screening criterion for the suitability of a deposition hole. Moreover, reproducing or predicting inflow may indicate whether a model reasonably represents flow processes in the fractured rock, with potential near-field modifications of properties. Estimating inflow is also essential as it determines water availability for bentonite hydration, and whether such wetting is controlled by the host rock or by the bentonite water-uptake capability.

The modelling groups calculated inflow into open boreholes for a large variety of conditions. In general, most modelling groups adjusted their models to improve the fit to the measured inflows, as discussed above. The calibration or conditioning efforts considerably narrowed the spread of reported inflow predictions, both within and between modelling groups. For example, the groups reported mean or median inflows between 0.08 and 0.46 ml/min, with minimum to maximum inflows ranging from 0.0 to 30 ml/min. Notably, some of the modelling groups reported very narrow ranges, suggesting high confidence in their predictions, whereas others provided wide ranges. In general, it appears difficult to blindly predict inflows from a fractured rock into an open borehole, i.e., models needed to be adjusted and calibrated to reproduce measured inflows. These adjustments not only required static characterisation data (such as stochastic fracture properties or fracture traces used for deterministic conditioning of the fracture networks at each of the boreholes), but also dynamic data, such as pressures and—specifically—inflow data, i.e., exactly the type of data for which predictions are to be made. Prediction ranges were relatively large, even if the models were conditioned and calibrated.

It is important to realize that the prediction of inflow into an open borehole may not be as critical for the prediction of bentonite wetting, as long as the order of magnitude of the inflow correctly identifies the dominant regime (i.e., whether water supply from the fractured rock is below or exceeds the water-uptake capacity of the bentonite).

Bentonite wetting time was selected as a performance measure because it is expected to be a key target prediction for numerical models that simulate the interaction between the natural and engineered barrier systems. The safety performance of the bentonite buffer partly depends on its swelling behaviour, which requires predicting the availability and uptake of sufficient formation water from the host rock.

The time until the entire bentonite buffer in a given borehole reaches a predefined average saturation was reported as the second performance measure. The importance of the location of fracture intersections (i.e., discrete inflow points) and the amount of water provided through the rock mass were universally recognized. Bentonite wetting times between less than one and more than 100 years were predicted. The range of wetting times reported by each modelling group is substantially narrower than the overall range obtained by combining the results from all modelling groups. All modelling groups reproduced the wetting time of the water-uptake test well. Predicting the idealized conditions of the WUT did not translate into similar wetting time predictions for the bentonite buffer in a larger deposition hole, which is highly determined by the location and geometry of discrete inflow points and water availability. Taken together, this demonstrates the relevance in field-scale investigations of using a multi-model approach that involves different modelling teams. The finding is, for instance, consistent with experiences from assessments of regional (hydro-)climatic change, where the benefits of using ensemble projections over individual model projections are well known (e.g., Jarsjö *et al.* 2012; Bring *et al.* 2015). Moreover, while the unique data set provided by the dismantling of BRIE significantly improved the fundamental understanding of the interface between the natural and engineered barrier systems, quantitative predictions of the data collected at sensors placed within the bentonite proved challenging.

The modelling groups' confidence in their predictions of bentonite wetting rests to a large degree on the favourable reproduction of data from the water-uptake test and the relative humidity data measured in the bentonite after BRIE dismantling.

Main interpretations and conclusions

As indicated above, differences in the conceptualization of the system and the implementation in a numerical model not only lead to differences in the predicted performance measures, but also to some disparities in interpretations and conclusions. This is expected as interpretations and conclusions are necessarily related to the conceptual model. Recognizing both consensus and disagreements about which features influence bentonite wetting and how well they are understood is an essential step towards the development of a defensible model prediction.

There was general consensus about the importance of the number, location, orientation, and properties of the discrete, water-conducting fractures that intersect the deposition holes, as they have a high impact on wetting patterns and bentonite hydration times. Mapping these fractures and deterministically implementing them into the model is essential for reliably predicting bentonite wetting. Furthermore, bentonite properties, specifically sorptivity (permeability and water retention curve) are key parameters. It seems to be possible to characterise or infer these properties with sufficient accuracy from laboratory tests of a single block (e.g., through a water-uptake test) despite them being emplaced as a stack of several blocks in the BRIE in situ experiments.

The second group of factors is related to the means by which water is carried to the deposition hole. The modelling groups' opinion on the relative importance of the fracture network versus that of the rock mass again reflects the chosen conceptual model. The modelling groups that developed a DFN considered the structure of the fracture network to be an essential component of the system that needs to be well understood to properly capture connectivity and water availability. These features are described using stochastic concepts; they thus have a random component that reflects spatial variability. It is noteworthy that this randomness is removed (even though the statistical metrics are preserved) at the interface itself, where mapped fractures are inserted deterministically. The modelling groups that developed an effective continuum model or a hybrid model concluded that the details of the far-field fracture network structure is of limited relevance and can thus be subsumed into a simplified continuum representation. Characterisation of the far field thus can be limited to a few effective properties that capture the formations ability to provide water to the region immediately surrounding the deposition holes. For dry sections of deposition holes that are not intersected by water-conducting features, the permeability of the rock mass (which may include microfractures) was considered important, but not explicitly included in the DFN models.

The third group of factors includes features that most modelling groups considered of limited importance. These factors included the large discrete features (deformation zones), which were generally considered of limited influence as long as they do not directly intersect a deposition hole or tunnel. The interface between the bentonite and the fractured rock was not explicitly considered in the modelling. For example, phenomena related to water movement from rock microstructure to bentonite interlayers and mineral surfaces were not taken into account. It can be assumed that the effects of phenomena specific to the rock-bentonite interface on the exchange of water from the natural to the engineered barrier system were either unknown or believed to be irrelevant. The details of the far-field boundary conditions were also considered insignificant as long as they supplied fluid and pressure support for the fractures carrying water to the deposition holes.

Both these agreements and discrepancies have to be considered when deciding what characterisation data are to be collected to improve the reliability of model predictions of bentonite wetting and ultimately deposition hole siting.

Characterisation and research needs

The prioritisation of characterisation and research needs is driven by the overall understanding of how the natural and engineered barrier systems interact with each other, and by the ranking of (uncertain) features that control bentonite wetting. The modelling groups generally agreed that bentonite properties can be sufficiently well characterized, i.e., residual uncertainty in predictions of bentonite wetting mainly result from uncertainties in the bedrock, specifically the fractures intersecting the deposition holes. Moreover, while the importance of fractures was recognized, it remains unclear which fracture characteristics need to be determined with high accuracy, and how they may be best included in a numerical model. Practical limitations (e.g., feasibility of detailed mappings of inflows or fractures intersecting probing holes) also need to be considered.

Despite some differences in the modelling groups' detailed views, it appears necessary to have sufficient characterisation data of the bentonite's water-uptake properties, and geometric and hydraulic properties of the local fractures intersecting the deposition hole. At the Äspö Hard Rock Laboratory, the network of intermediate-scale fractures seems sufficiently connected to provide water to the deposition holes in amounts exceeding the demand of the bentonite; consequently, a simplified representation of the far field appears justified at this specific site.

Coupled processes were deliberately excluded from this Task Force study in both the field experiment (BRIE was designed as an experiment without mimicking the thermal output of high-level radioactive waste), and the numerical modelling, which focused on hydrological processes. It was fully recognized that the exclusion of coupled THMC processes limited the ability of the models to explain and reproduce the field data, or to predict relevant system behaviour. However, it should be noted that there are considerable conceptual and quantitative uncertainties in the THMC coupling terms. The need to include complex coupled processes into numerical models (a topic of active research) should thus be assessed in the light of the specific technical question being addressed.

Concluding remarks

The main purpose of the Task 8 studies was to improve overall understanding of the water exchange between the natural and engineered barrier systems. Based on this improved understanding, secondary objectives can be achieved. In particular, characterisation methods are to be developed that help modellers improve their predictions of bentonite wetting times, which can then be used to establish deposition hole criteria.

One of the most beneficial outcomes of Task 8 is the large number of alternative conceptual models that were developed to address a common issue based on a common set of characterisation data and background information. The variety of approaches taken to assess the interaction between the fractured rock and the bentonite buffer in a deposition hole led to insights and conclusions that can be considered robust in cases where different groups converged on a consistent understanding, and highlight fundamental uncertainties, ambiguities, or lack of defensible understanding in cases where opposing views were held despite the common information available to and shared among the modelling groups. Both of these types of insights are equally valuable.

In particular, the range of predicted bentonite wetting times obtained in individual models were considerably narrower than the range encompassed by the ensemble results of all models. This was not the case when the same models were applied to more well-defined laboratory set-ups, hence reflecting an on-set of conceptual uncertainty impacts in larger (field scale) applications. More generally, these results demonstrate the relevance of using a multi-model approach that involves different modelling teams in field-scale hydrogeological applications. Thus far, such practice is uncommon in the field of hydrogeology, although the considerable benefits of ensemble model results over individual model results are well known for Earth system model projections of regional (hydro-)climatic change.

Conceptual understanding evolved during the modelling exercise of Task 8. Interestingly, this does not necessarily lead to a reduction in conceptual model uncertainty, as new features were detected, or their relevance for predicting bentonite wetting had to be updated. As the ranking of features changes, so does the accuracy with which they need to be characterized. An example is the need to accurately map discrete features intersecting and providing water to a deposition hole; the need for such specific information goes beyond a stochastic description of the fracture network.

Conceptual uncertainty remains difficult to assess even if multiple alternative models are available for comparison. There are multiple reasons for this, among which is the fact that conceptual models are often developed within the framework and constraints of the available simulation tools rather than based on a critical assessment of key features and processes. Alternative conceptual models also overlap considerably and in significant aspects (notably the use of a common set of incomplete characterisation data, or the use of identical or very similar governing equations); they thus do not produce the spread of results one would expect from truly independent conceptualizations. Calibration of models against a common set of observations partly absorbs conceptual modelling errors; however, this benefit does not necessarily translate into a higher reliability in model predictions. Finally, the universe of possible conceptual models is essentially infinite, making it impossible to examine a sufficient number of viable alternatives.

The importance of fractures for understanding and predicting fluid flow and bentonite hydration is universally recognized. Nevertheless, there remain considerable differences in the assessment of which properties of fractures and fracture networks are most essential, how to best characterize them, and how to properly include them in a representative and efficient manner in a numerical model. The differences in the modelling groups' view are essential, as they determine the choice of (potentially costly) characterization methods and modelling approaches.

As uncertainties and errors in the conceptualisation of complex systems are unavoidable, the question arises to which extent decisions should be based on modelling results or site-specific data. It became evident that deposition hole siting decisions will need to be based on both local characterisation data and some (potentially simplified) predictive modelling.

Finally, the availability of multiple conceptual models focussed on shared objectives provided a wider set of constructs (e.g. the nearfield/farfield split in the hybrid models) with which to consider system behaviour and to generalise the results to repository conditions.

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Figure Captions

Fig. 1. The BRIE site in the TASO tunnel: drilling of the 300 mm boreholes (left), emplacement of the 3 m bentonite blocks (middle), extraction of bentonite blocks after 17 months (right) (source: Fransson *et al.* 2017).

Fig. 2. Schematic and photograph of the BRIE water-uptake test. Water is introduced via the outer cylindrical filter. The 100 mm bentonite block is identical in material to the stack of blocks emplaced in the BRIE in situ experiments (Fig. 1) (source: Fransson *et al.* 2017).

Fig. 3. Schematic of key system elements, processes, and modelling issues related to the interaction between fractured diorite and a bentonite-filled surrogate deposition at the Äspö Hard Rock Laboratory, Sweden.

Fig. 4. Alternative representations of fractured rock: (**a**) classical discrete fracture network model, (**b**) heterogeneous effective continuum model with deterministic fractures around boreholes, (**c**) hybrid DFN-continuum model, and (**d**) model with artificial fractures and skin zones.

Fig. 5. Examples of the use of characterization and monitoring data: (**a**) reproducing relative humidity data; (**b**), conditioning of fracture locations and orientations; (**c**) selection of DFN realization that best reproduces inflow into open surrogate deposition hole.

Fig. 6. Comparison between measured and calculated (**a**) cumulative water uptake, (**b**) relative humidity, and (**c**) saturation for the WUT.

Fig. 7. Simulated (left) and observed (right) wetting patterns at the interface between fracture rock and the bentonite buffer.

Fig. 8. Saturation distributions in bentonite calculated using different conceptual models.